

1 What is claimed is:

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1 1. A computer-implemented method for generating a library design for a combinatorial
2 library of materials, comprising:

3 defining one or more sources and one or more destinations, each source being
4 electronic data representing a component to be used in preparing the combinatorial library
5 and each destination being electronic data representing an arrangement of cells;

6 receiving an input defining a first mapping, the first mapping being electronic data
7 defining a distribution pattern for assigning a component to cells in the arrangement, the
8 distribution pattern including a minimum and a maximum amount of the component to be
9 assigned to any cell of the arrangement and a gradient to be applied between the minimum
10 and maximum amounts of the component across the plurality of cells;

11 using the first mapping to calculate a composition of one or materials assigned to one
12 or more of the cells; and

13 generating a data file defining the library design, the data file comprising electronic
14 data representing the sources, the destinations and the mapping.

1 2. The method of claim 1, further comprising:

2 displaying a representation of the library design, the representation graphically
3 describing the composition of one or more materials assigned to one or more of the cells.

1 3. The method of claim 1, wherein the data file comprises electronic data representing
2 one or more sets of properties, each set of properties being associated with one of the
3 sources, the destinations or the mapping.

1 4. The method of claim 1, wherein defining the sources and destinations comprises
2 receiving an input from a graphical input device.

1 5. The method of claim 1, wherein the input defining a first mapping comprises a
2 selection from a set of available mapping types, the set of available mapping types
3 comprising a one to one mapping of a component from a source to a cell in the arrangement
4 and a one to many mapping of a component from a source to a plurality of cells in the
5 arrangement.

1 6. The method of claim 5, wherein the set of available mapping types further comprises
2 a many to many mapping of a plurality of components from a plurality of sources to a
3 plurality of cells in the arrangement.

1 7. The method of claim 6, wherein the set of available mapping types further comprises
2 a many to one mapping of a plurality of components from a plurality of sources to a cell in
3 the arrangement.

1 8. The method of claim 5, wherein the set of available mapping types further comprises
2 a set of one or more user-defined equations.

1 9. The method of claim 1, wherein the gradient is selected from the group consisting of
2 linear, logarithmic, exponential, polynomial and geometric progression.

1 10. The method of claim 3, wherein the set of properties associated with the mapping
2 comprises a source name, a source geometry, a destination name, a destination geometry, a
3 gradient type, and a set of gradient parameters defining the gradient.

1 11. The method of claim 1, further comprising:

2 receiving an input defining a second mapping, the second mapping being electronic
3 data defining a second distribution pattern for distributing a second component to cells in the
4 arrangement; and

5 using the first and second mappings to calculate a composition of one or more
6 materials assigned to one or more of the cells.

1 12. The method of claim 11, wherein the second distribution pattern for assigning a
2 second component includes electronic data identifying a fixed amount of the second
3 component to be assigned to one or more cells in the arrangement.

1 13. The method of claim 12, wherein the second distribution pattern for assigning a
2 second component includes electronic data identifying a minimum and a maximum amount
3 of the second component to be assigned to any of the cells of the arrangement and a second
4 gradient to be applied between the minimum and maximum amounts of the second
5 component across the cells.

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1 14. The method of claim 1, further comprising generating a modified library design by:
2 receiving an input redefining a source, a destination or a mapping;
3 recalculating the composition of one or more materials assigned to one or more of the
4 cells; and
5 generating a data file defining the modified library design.

1 15. The method of claim 1, further comprising:
2 receiving an input defining one or more parameters, each parameter being electronic
3 data corresponding to a process parameter and defining a parameter value for one or more
4 cells of the arrangement, the parameter value varying between a minimum and a maximum
5 amount; and
6 wherein the data file further comprises electronic data representing the one or more
7 parameters.

1 16. The method of claim 1, wherein the arrangement comprises two or more cells.

1 17. The method of claim 1, wherein the arrangement comprises ten or more cells.

1 18. The method of claim 1, wherein the arrangement comprises about ninety-six or more
2 cells.

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1 19. A computer-implemented method for generating a library design for a combinatorial
2 library of materials, comprising:
3 defining a set of one or more sources and one or more destinations, each source being
4 electronic data representing a component to be used in preparing the combinatorial library
5 and each destination being electronic data representing an arrangement of cells;
6 receiving an input defining a set of first mappings, the first mappings being electronic
7 data defining a set of equations for calculating an amount of one or more components to be
8 assigned to one or more cells in an arrangement;
9 using the set of equations to calculate a composition of a material assigned to one or
10 more of the cells; and
11 generating a data file defining the library design, the data file comprising electronic

1285 data representing the sources, the destinations and the mappings.

1 20. The method of claim 19, further comprising:
2 displaying a representation of the library design, the representation graphically
3 describing the composition of one or more materials assigned to one or more of the cells.

1 21. The method of claim 19, wherein the component to be assigned to a cell in the
2 arrangement is determined by the location of the cell within the arrangement.

1 22. The method of claim 21, wherein the composition of a material is determined using a
2 subset of the set of equations, the subset of equations being determined by the location of the
3 cell within the arrangement.

1 23. The method of claim 19, further comprising:
2 generating an error indicator signal if the number of equations in the set of equations
3 is not equal to the number of sources in the set of sources.

1 24. The method of claim 19, wherein at least one of the set of equations is selected from
2 the group consisting of:

3 a ratio equation defining an amount of a component to be assigned to a cell as a
4 function of an amount of another component to be assigned to the cell;

5 a volume equation defining an amount of a component to be assigned to a cell as a
6 function of a total volume of a plurality of components to be assigned to the cell; and

7 a mass equation defining an amount of a component to be assigned to a cell as a
8 function of a total mass of a plurality of components to be assigned to the cell.

1 25. The method of claim 19, wherein the set of equations comprises a gradient equation
2 defining an amount of a component to be assigned to each of a plurality of cells according to
3 a gradient.

1 26. The method of claim 19, wherein each of the set of equations is assigned to one or
2 more cells of the arrangement according to the location of the cells within the arrangement.

1 27. The method of claim 19, wherein using the set of equations to calculate a composition
2 of a material assigned to one or more of the cells comprises simultaneously solving a set of
3 interdependent equations.

1 28. The method of claim 27, wherein using the set of equations further comprises using a
2 matrix inversion technique to solve the set of equations.

1 29. The method of claim 19, further comprising:

2 receiving an input defining a second mapping, the second mapping being electronic
3 data defining a distribution pattern for distributing a component to cells in the arrangement,
4 the distribution pattern including a minimum and a maximum amount of the component to be
5 assigned to any cell of the cells of the arrangement and a gradient to be applied between the
6 minimum and maximum amounts of the component across the plurality of cells; and

7 using the first set of mappings and the second mapping to calculate a composition of
8 a material assigned to one or more of the cells.

1 Sub 30. A computer-implemented method for generating a library design for a combinatorial
2 B6 library of materials, comprising:

3 defining a set of one or more sources and one or more destinations, each source being
4 electronic data representing a component to be used in preparing the combinatorial library
5 and each destination being electronic data representing an arrangement of cells;

6 defining a plurality of mappings, the mappings in the aggregate defining a
7 composition for each of a plurality of materials assigned to a plurality of cells in the
8 arrangement;

9 receiving an input defining one or more parameters, each parameter being electronic
10 data corresponding to a process parameter and defining a parameter value for one or more
11 cells of the arrangement, the parameter value varying between a minimum and a maximum
12 amount; and

13 generating a data file defining the library design, the data file comprising electronic
14 data describing the source elements, the destination elements, the mappings and the
15 parameters.

1 31. The method of claim 30, wherein the parameter value is defined to vary over time.

2 32. The method of claim 30, wherein the parameter value is defined to vary across two or
3 more cells in the arrangement.

4 33. The method of claim 30, wherein the parameter value is defined to vary over time and

5 across two or more cells in the arrangement.

1 34. The method of claim 30, wherein the parameter value varies according to a gradient
2 selected from the group consisting of linear, logarithmic, exponential, polynomial and
3 geometric progression.

1 35. The method of claim 30, wherein the parameter value corresponds to a process
2 parameter selected from the group consisting of temperature, pressure, time, flow rate and
3 stirring speed.

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1 36. A computer-implemented method for preparing a combinatorial library of materials
2 on a substrate, the method comprising:

3 creating a library design by defining a set of design elements, the set of design
4 elements including one or more sources representing components to be used in preparing the
5 combinatorial library, one or more destinations, each destination comprising an arrangement
6 of one or more cells, and one or more elements selected from the group consisting of a
7 mapping defining a scheme for assigning one or more amounts of a component to one or
8 more cells of an arrangement and a parameter corresponding to a process parameter, the
9 parameter defining a parameter value for one or more cells of the arrangement, the parameter
10 value varying between a minimum and a maximum amount;

11 generating a data file comprising electronic data describing the sources, the
12 destinations, the mappings and the parameters; and

13 using the data file to cause an automated material handling apparatus to assemble the
14 combinatorial library on a substrate.

1 37. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 receive an input defining one or more sources and one or more destinations, each
5 source being electronic data representing a component to be used in preparing the
6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;

8 receive an input defining a first mapping, the first mapping being electronic data
9 defining a distribution pattern for assigning a component to cells in the arrangement, the

10 distribution pattern including a minimum and a maximum amount of the component to be
11 assigned to any cell of the arrangement and a gradient to be applied between the minimum
12 and maximum amounts of the component across the plurality of cells;

13 *B7* use the first mapping to calculate a composition of one or materials assigned to one or
14 more of the cells; and

15 generate a data file defining the library design, the data file comprising electronic data
16 representing the sources, the destinations and the mapping.

1 38. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 display a representation of the library design, the representation graphically
4 describing the composition of one or more materials assigned to one or more of the cells.

1 39. The computer program of claim 37, wherein the data file comprises electronic data
2 representing one or more sets of properties, each set of properties being associated with one
3 of the sources, the destinations or the mapping.

1 40. The computer program of claim 37, wherein the input defining the sources and
2 destinations comprises an input from a graphical input device.

1 41. The computer program of claim 37, wherein the input defining a first mapping
2 comprises a selection from a set of available mapping types, the set of available mapping
3 types comprising a one to one mapping of a component from a source to a cell in the
4 arrangement and a one to many mapping of a component from a source to a plurality of cells
5 in the arrangement.

1 42. The computer program of claim 41, wherein the set of available mapping types
2 further comprises a many to many mapping of a plurality of components from a plurality of
3 sources to a plurality of cells in the arrangement.

1 43. The computer program of claim 42, wherein the set of available mapping types
2 further comprises a many to one mapping of a plurality of components from a plurality of
3 sources to a cell in the arrangement.

1 44. The computer program of claim 40, wherein the set of available mapping types

2 further comprises a set of one or more user-defined equations.

1 45. The computer program of claim 37, wherein the gradient is selected from the group
2 consisting of linear, logarithmic, exponential, polynomial and geometric progression.

1 46. The computer program of claim 39, wherein the set of properties associated with the
2 mapping comprises a source name, a source geometry, a destination name, a destination
3 geometry, a gradient type, and a set of gradient parameters defining the gradient.

1 47. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 receive an input defining a second mapping, the second mapping being electronic
4 data defining a second distribution pattern for distributing a second component to cells in the
5 arrangement; and

6 use the first and second mappings to calculate a composition of one or more materials
7 assigned to one or more of the cells.

1 48. The computer program of claim 47, wherein the second distribution pattern for
2 assigning a second component includes electronic data identifying a fixed amount of the
3 second component to be assigned to one or more cells in the arrangement.

1 49. The computer program of claim 48, wherein the second distribution pattern for
2 assigning a second component includes electronic data identifying a minimum and a
3 maximum amount of the second component to be assigned to any of the cells of the
4 arrangement and a second gradient to be applied between the minimum and maximum
5 amounts of the second component across the cells.

1 50. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to generate a modified library design by receiving an input
3 redefining a source, a destination or a mapping; recalculating the composition of one or more
4 materials assigned to one or more of the cells; and generating a data file defining the
5 modified library design.

1 51. The computer program of claim 37, further comprising instructions operable to cause
2 a programmable processor to:

3 receive an input defining one or more parameters, each parameter being electronic
4 data corresponding to a process parameter and defining a parameter value for one or more
5 cells of the arrangement, the parameter value varying between a minimum and a maximum
6 amount; and

7 wherein the data file further comprises electronic data representing the one or more
8 parameters.

1 *B1* 52. The computer program of claim 37, wherein the arrangement comprises two or more
2 cells.

1 53. The computer program of claim 37, wherein the arrangement comprises ten or more
2 cells.

1 54. The computer program of claim 37, wherein the arrangement comprises about ninety-
2 six or more cells.

1 55. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 receive an input defining a set of one or more sources and one or more destinations,
5 each source being electronic data representing a component to be used in preparing the
6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;

8 receive an input defining a set of first mappings, the first mappings being electronic
9 data defining a set of equations for calculating an amount of one or more components to be
10 assigned to one or more cells in an arrangement;

11 use the set of equations to calculate a composition of a material assigned to one or
12 more of the cells; and

13 generate a data file defining the library design, the data file comprising electronic data
14 representing the sources, the destinations and the mappings.

1 56. The computer program of claim 55, further comprising instructions operable to:

2 display a representation of the library design, the representation graphically
3 describing the composition of one or more materials assigned to one or more of the cells.

1 57. The computer program of claim 55, wherein the component to be assigned to a cell in
2 the arrangement is determined by the location of the cell within the arrangement.

1 58. The computer program of claim 57, wherein the composition of a material is
2 determined using a subset of the set of equations, the subset of equations being determined
3 by the location of the cell within the arrangement.

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1 59. The computer program of claim 55, further comprising instructions operable to:
2 generate an error indicator signal if the number of equations in the set of equations is
3 not equal to the number of sources in the set of sources.

1 60. The computer program of claim 55, wherein at least one of the set of equations is
2 selected from the group consisting of:

3 a ratio equation defining an amount of a component to be assigned to a cell as a
4 function of an amount of another component to be assigned to the cell;

5 a volume equation defining an amount of a component to be assigned to a cell as a
6 function of a total volume of a plurality of components to be assigned to the cell; and

7 a mass equation defining an amount of a component to be assigned to a cell as a
8 function of a total mass of a plurality of components to be assigned to the cell.

1 61. The computer program of claim 55, wherein the set of equations comprises a gradient
2 equation defining an amount of a component to be assigned to each of a plurality of cells
3 according to a gradient.

1 62. The computer program of claim 55, wherein each of the set of equations is assigned
2 to one or more cells of the arrangement according to the location of the cells within the
3 arrangement.

1 63. The computer program of claim 55, wherein the instructions operable to cause a
2 programmable processor to use the set of equations to calculate a composition of a material
3 assigned to one or more of the cells comprise instructions simultaneously to solve a set of
4 interdependent equations.

1 64. The computer program of claim 63, wherein the instructions simultaneously to solve
2 the set of interdependent equations further comprise instructions to use a matrix inversion

3 technique to solve the set of equations.

1 65. The computer program of claim 55, further comprising instructions operable to:

2 receive an input defining a second mapping, the second mapping being electronic

3 data defining a distribution pattern for distributing a component to cells in the arrangement,

4 the distribution pattern including a minimum and a maximum amount of the component to be

5 assigned to any cell of the cells of the arrangement and a gradient to be applied between the

6 minimum and maximum amounts of the component across the plurality of cells; and

7 use the first set of mappings and the second mapping to calculate a composition of a

8 material assigned to one or more of the cells.

1 66. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 receive an input defining a set of one or more sources and one or more destinations,

5 each source being electronic data representing a component to be used in preparing the

6 combinatorial library and each destination being electronic data representing an arrangement
7 of cells;

8 receive an input defining a plurality of mappings, the mappings in the aggregate
9 defining a composition for each of a plurality of materials assigned to a plurality of cells in
10 the arrangement;

11 receive an input defining one or more parameters, each parameter being electronic
12 data corresponding to a process parameter and defining a parameter value for one or more
13 cells of the arrangement, the parameter value varying between a minimum and a maximum
14 amount; and

15 generate a data file defining the library design, the data file comprising electronic data
16 describing the source elements, the destination elements, the mappings and the parameters.

1 67. The computer program of claim 66, wherein the parameter value is defined to vary
2 over time.

1 68. The computer program of claim 66, wherein the parameter value is defined to vary
2 across two or more cells in the arrangement.

1 69. The computer program of claim 66, wherein the parameter value is defined to vary
2 B7 over time and across two or more cells in the arrangement.

1 70. The computer program of claim 66, wherein the parameter value varies according to a
2 gradient selected from the group consisting of linear, logarithmic, exponential, polynomial
3 and geometric progression.

1 71. The computer program of claim 66, wherein the parameter value corresponds to a
2 process parameter selected from the group consisting of temperature, pressure, time, flow
3 rate and stirring speed.

1 72. A computer program product on a computer-readable medium for generating a library
2 design for a combinatorial library of materials, the program comprising instructions operable
3 to cause a programmable processor to:

4 create a library design by defining a set of design elements, the set of design elements
5 including one or more sources representing components to be used in preparing the
6 combinatorial library, one or more destinations, each destination comprising an arrangement
7 of one or more cells, and one or more elements selected from the group consisting of a
8 mapping defining a scheme for assigning one or more amounts of a component to one or
9 more cells of an arrangement and a parameter corresponding to a process parameter, the
10 parameter defining a parameter value for one or more cells of the arrangement, the parameter
11 value varying between a minimum and a maximum amount;

12 generate a data file comprising electronic data describing the sources, the
13 destinations, the mappings and the parameters; and

14 use the data file to cause an automated material handling apparatus to assemble the
15 combinatorial library on a substrate.